# Exact Solutions of Domain Wall and Spiral Ground States in Hubbard Models

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We construct a set of exact ground states with a localized ferromagnetic domain wall and an extended spiral structure in a deformed flat-band Hubbard model. In the case of quarter filling, we show the uniqueness of the ground state with a fixed magnetization. We discuss a more realistic situation given by a band-bending perturbation, which can stabilize these curious structures. We study a conduction electron scattered by the domain wall and the spiral spins.

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Domain wall and spiral structures in ferromagnetic systems are interesting structures. Generally a domain wall is localized stably between two ferromagnetic domains. In this case, the ferromagnetic order is preserved within one domain, and the translational symmetry is spontaneously broken. Domain structures are believed to appear universally in ferromagnetic systems with an energy gap and with a finite correlation length. On the other hand, spiral structures appear in special situations. Such structures are extended over the entire space, and sometimes destroy ferromagnetic order. In this letter, we construct a set of exact ground states in a class of Hubbard-like models with coexisting domain wall and spiral structures, which have never been found in other models. Some remarkable results for ferromagnetic ground states have been obtained in a class of Hubbard models recently. Mielke and Tasaki showed independently that the ground state gives saturated ferromagnetism in a many-electron model on a lattice with special properties, which is called the flat-band Hubbard model [1, 2]. Tasaki also proved the stability of the ferromagnetism against a perturbation which bends the electron band [3]. Tanaka and Ueda have shown this stability for a two-dimensional model in Mielke's class [4]. If domain wall structures are universal, then a domain wall solution within this framework should give us some important physical insight into theories of many-electron systems. Here, we construct such a solution. We deform a flat-band Hubbard model by introducing a complex anisotropy parameter $q$. The SU(2) spin rotation symmetry in the original flat-band model is reduced to U(1) in our deformed model. This anisotropy $|q| \neq 1$ leads to a localized domain wall with a finite width and a complex $q$ leads to an extended spiral state. We study the stability of the domain wall ground states against a band-bending perturbation using a variational argument. We prove that for $|q| \neq 1$, the energy expectation value of a state with a domain wall centered near the origin becomes lower than the eigenvalue of the saturated ferromagnetic eigenstate, unlike the SU(2) invariant model. We discuss similarities of the wall solution and differences between the domain wall solution of our model and domain walls in pure quantum spin systems. Alcaraz, Salinas and Wreszinski constructed a set of exact ground states with two domains in the XXZ model with a critical boundary field in arbitrary dimensions for an arbitrary spin [5]. They showed that the degeneracy of the ground states corresponding to the location of a domain wall center is identical to that of the ground states in the SU(2) invariant model. In their solution, the domain wall is localized at an arbitrary surface with a finite width depending on the Ising anisotropy parameter $(q+q^{-1})/2 > 1$. We will see that the domain wall ground state in our electron model has the same degeneracy as that in the XXZ model and the same localization property in a certain parameter regime. On the other hand, for complex $q$, our model differs from the XXZ quantum spin model which has no spiral ground state. Finally, we study from a microscopic viewpoint the scattering of a conduction electron by the domain wall and spiral spins.

Here, we consider a one-dimensional lattice with a site index $x = -L-1, \cdots, L+1$, where $x$ is an integer and $L$ is an odd integer. Electron operators on the lattice satisfy the anticommutation relation

$$\{c_{x\sigma}, c^\dagger_{y\tau}\} = \delta_{\sigma\tau}\delta_{xy}, \quad \sigma,\tau = \uparrow,\downarrow .$$

We define the following electron operators for even site $x$ with a complex number $q$ and a real number $\lambda > 0$

$$\begin{aligned}
a_{x-1\uparrow} &\equiv -(q^{1/4})^* c_{x-2\uparrow} + \lambda c_{x-1\uparrow} - (q^{-1/4})^* c_{x\uparrow}, \\
a_{x-1\downarrow} &\equiv -(q^{-1/4})^* c_{x-2\downarrow} + \lambda c_{x-1\downarrow} - (q^{1/4})^* c_{x\downarrow}, \\
d_{x\uparrow} &\equiv q^{-1/4} c_{x-1\uparrow} + \lambda c_{x\uparrow} + q^{1/4} c_{x+1\uparrow}, \\
d_{x\downarrow} &\equiv q^{1/4} c_{x-1\downarrow} + \lambda c_{x\downarrow} + q^{-1/4} c_{x+1\downarrow}, \qquad (1)\\
n_{x\uparrow} &\equiv c^\dagger_{x\uparrow} c_{x\uparrow}, \quad n_{x\downarrow} \equiv c^\dagger_{x\downarrow} c_{x\downarrow}, \quad n_x \equiv n_{x\uparrow} + n_{x\downarrow}. \qquad (2)
\end{aligned}$$

The operators $a_{x\sigma}$ and $d^\dagger_{y\tau}$ are always anticommuting

$$\{a_{x\sigma}, d^\dagger_{y\tau}\} = 0, \quad x = \text{odd},\ y = \text{even}, \quad \sigma,\tau = \uparrow,\downarrow . \qquad (3)$$

The Hamiltonian is written in terms of the above opera-

tors as

$$H = H_{\rm hop} + H_{\rm int} \tag{4}$$

$$H_{\rm hop} = t \sum_{x={\rm even}} (d^\dagger_{x\uparrow} d_{x\uparrow} + d^\dagger_{x\downarrow} d_{x\downarrow}) = \sum_{x,y,\sigma} t^\sigma_{xy} c^\dagger_{x\sigma} c_{y\sigma} \tag{5}$$

$$H_{\rm int} = U \sum_x n_{x\uparrow} n_{x\downarrow}, \tag{6}$$

with a repulsive coupling constant $U > 0$ and a hopping parameter $t > 0$. The anticommutativity and the absence of $a_{x\sigma}$ in $H_{\rm hop}$ give a band flatness of the electrons created by $a^\dagger_{x\sigma}$. Here we use an open-boundary condition under which there are no degrees of freedom at the edge sites $x = -L-2$ and $x = -L+2$, namely $c_{-L-2\sigma} = 0 = c_{L+2\sigma}$. The hopping amplitudes on a unit cell defined by $H_{\rm hop}$ are depicted in Fig. 1.

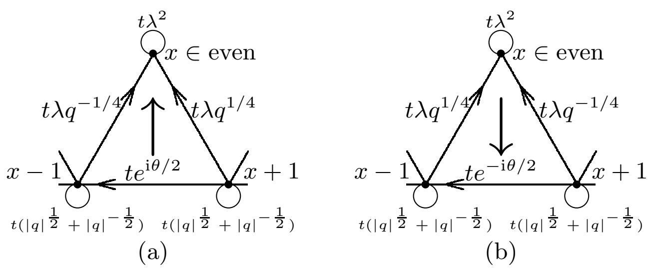


FIG. 1: Arrows and circles depict hopping amplitudes and on-site potentials, respectively, for electrons with up(a) and down(b) spins on a unit cell. For complex $q = |q|e^{{\rm i}\theta}$, the hopping amplitude opposite to the arrow is the complex conjugate of that along the arrow.

Let us discuss the symmetry of this Hamiltonian. The first important symmetry is U(1) symmetry. The Hamiltonian commutes with the total magnetization $S^{(3)}$, where we define $S^{(j)} \equiv \sum_x S^{(j)}_x$ and $S^{(j)}_x \equiv \frac{1}{2}\sum_{\alpha,\beta=\uparrow,\downarrow} c^\dagger_{x\alpha}\sigma^{(j)}_{\alpha\beta}c_{x\beta}$, where $\sigma^{(j)}$ $(j = 1, 2, 3)$ are the Pauli matrices. In the limit $q \to 1$, this symmetry is enhanced to the SU(2) symmetry. In this limit, this model becomes the original flat-band Hubbard model given by Tasaki [2, 3]. The second important symmetry is defined by a product of a parity $P$ and a spin rotation

$$\Pi = \Pi^{-1} = P \exp\left({\rm i}\pi S^{(1)}\right) \tag{7}$$

$$\Pi c_{x\sigma} \Pi = c_{-x\ -\sigma}, \Pi c^\dagger_{x\sigma}\Pi = c^\dagger_{-x\ -\sigma},$$

Note the following transformation of the total magnetization $\Pi S^{(3)}\Pi = -S^{(3)}$. An energy eigenstate with the total magnetization $M$ is transformed by $\Pi$ into another eigenstate with the total magnetization $-M$, which belongs to the same energy eigenvalue.

Now we construct ground states in the quarter-filled case, where the uniqueness of the ground state can be shown. Since each term in the Hamiltonian is positive semi-definite $H_{\rm hop} \geq 0$ and $H_{\rm int} \geq 0$, an eigenstate with a zero-energy eigenvalue is a ground state. An arbitrary state created only by $a^\dagger_{x\uparrow}$ is a zero-energy states because of its anticommutativity (3) with $d_{x\uparrow}$ and no double occupancy, and thus this polarized state

$$|{\rm all\ up}\rangle = \prod_{x={\rm odd}} a^\dagger_{x\uparrow}|{\rm vac}\rangle, \tag{8}$$

is a ground state. To create ground states with other magnetization, first we should take into account a condition of no double occupancy at odd sites. A state created by $a^\dagger_{x\sigma}$ under this condition is written in the following summation over all spin configurations with an arbitrary fixed magnetization $\sum_x \sigma_x = M$

$$|M\rangle = \sum_{\sigma_{-L}+\cdots+\sigma_L = M} \psi(\sigma_{-L}, \cdots, \sigma_L) \prod_{x={\rm odd}} a^\dagger_{x\sigma_x}|{\rm vac}\rangle.$$

The condition of no double occupancy on the state $|M\rangle$ at even sites yields

$$\psi(\cdots, \uparrow, \downarrow, \cdots) = q\ \psi(\cdots, \downarrow, \uparrow, \cdots).$$

This relation implies the uniqueness of the ground state with a fixed total magnetization, since two arbitrary spin configurations can be related by the successive exchanges of two nearest neighbor spins. Therefore the degeneracy of those ground states is exactly the same as that in the SU(2) symmetric model, as in the domain wall solution in quantum spin systems [5].

To explore the nature of the ground state, we write it in a more explicit way. The following superposition over the states with different magnetizations can be a ground state

$$|z\rangle \equiv \sum_M z^{L-M}|M>= \prod_{x={\rm odd}} (a^\dagger_{x\uparrow} + zq^{\frac{x}{2}} a^\dagger_{x\downarrow})|{\rm vac}\rangle,, \tag{9}$$

where $z$ is an arbitrary complex number. This state can be regarded as a generating function for a ground state with an arbitrary magnetization. The expectation values

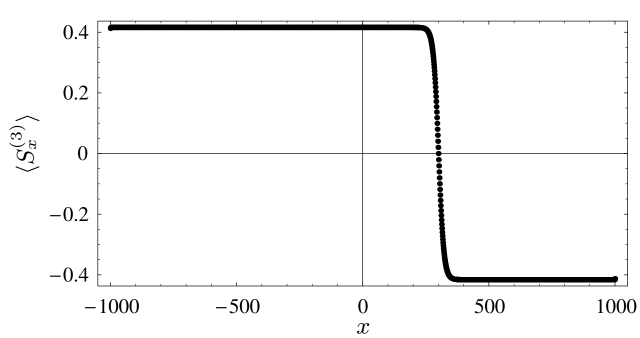


FIG. 2: Spin one point function on odd sites $x$ evaluated from the numerical solution of the recursion relation for $L = 1000$, $q = 1.05$, $\lambda = 3$ and $z = 1.05^{-300}$.

of the spin operators at site $x$ in this ground state are

$$\left\langle S_x^{(1)}\right\rangle = \frac{\langle n_x\rangle}{2}\frac{zq^{\frac{x}{2}}+(zq^{\frac{x}{2}})^*}{1+|z^2q^x|}$$
$$\left\langle S_x^{(2)}\right\rangle = \frac{\langle n_x\rangle}{2\mathrm{i}}\frac{zq^{\frac{x}{2}}-(zq^{\frac{x}{2}})^*}{1+|z^2q^x|}$$
$$\left\langle S_x^{(3)}\right\rangle = \frac{\langle n_x\rangle}{2}\frac{1-|z^2q^x|}{1+|z^2q^x|}, \tag{10}$$

where the expectation value of an operator $\mathcal{O}$ is defined by $\langle\mathcal{O}\rangle \equiv \langle z|\mathcal{O}|z\rangle/\langle z|z\rangle$. As discussed in the XXZ models [6, 7, 8, 9], the two domains are distinguished by the sign of the local order parameter $\langle S_x^{(3)}\rangle$. The domain wall center is defined by the zeros of $\langle S_x^{(3)}\rangle$ which is located at $x=-2\log_{|q|}|z|$. The function $\frac{1}{2}\langle n_x\rangle - |\langle S_x^{(3)}\rangle|$ decays exponentially from the center, if $\langle n_x\rangle \neq 0$. The domain wall width $1/\log|q|$ is defined by its decay length. A profile of the domain wall in a typical example is depicted in Fig.2. For the complex $q=|q|e^{\mathrm{i}\theta}$, one can see the spiral structure with a pitch angle $\theta$. The vector $\langle\vec{S}_x\rangle$ is rotated with angle $\theta x$ around the third spin axis depending on the site $x$. Note that this spiral structure of the ground state does not exist in the XXZ model. Though the complex anisotropy parameter $q=e^{\mathrm{i}\theta}$ is possible in the XXZ Hamiltonian, the spiral state is no longer the ground state and the corresponding model is described in the Tomonaga-Luttinger liquid without ferromagnetic order. The translational symmetry in the infinite volume limit is broken by the domain wall or the spiral structure for finite $\log|z|$. Both symmetries generated by $S^{(3)}$ and $\Pi$ are broken spontaneously as well.

Now, we evaluate the function $\langle n_x\rangle$ to see the practical form of $\langle\vec{S}_x\rangle$ given by eq. (10). First we consider a simple case of the large $\lambda$ limit. This limit implies that there is no overlapping of the electrons at each even site, thus

$$\langle n_x\rangle = 1-O(\lambda^{-2}),\ x=\text{odd},\ \ \langle n_x\rangle = O(\lambda^{-2}),\ x=\text{even}. \tag{11}$$

The localization property of the ground state in this case is the same as in the XXZ model. To treat a general case, we introduce the following normalization function

$$A(x_0,x,\zeta) \equiv \|\prod_{y=x_0}^{x}(a_{y\uparrow}^\dagger + |q|^{-\frac{\zeta}{2}}q^{\frac{y}{2}}a_{y\downarrow}^\dagger)|\mathrm{vac}\rangle\|^2, \tag{12}$$

where we employ $z$ as a real number and use a parameterization $z^2=|q|^{-\zeta}$ for $|q|>1$. Note $A(-L,L,\zeta)=\langle z|z\rangle$. This normalization function obeys the recursion relation

$$\begin{aligned} A(x_0,x,\zeta) =&\epsilon\ (1+|q^{x-\zeta}|)A(x_0,x-2,\zeta) \\ &-(1+|q^{x-\zeta-1}|)^2A(x_0,x-4,\zeta), \end{aligned} \tag{13}$$

where $\epsilon \equiv \lambda^2+|q|^{1/2}+|q|^{-1/2}$. We can extract the main $x$ dependent part out of $A(x_0,x,\zeta)$ as follows

$$A(x_0,x,\zeta) = B(x_0,x,\zeta)r^{\frac{x-x_0+2}{2}}\prod_{y=x_0}^{x}(1+|q^{y-\zeta}|), \tag{14}$$

where $r\equiv(\epsilon+\sqrt{\epsilon^2-4})/2$. The convergence of the quotient $B(-L,x,\zeta)$ in the infinite volume limit is proved rigorously on the basis of the recursion relation for $B(-L,x,\zeta)$ derived from the recursion relation (13) [10]. The one point function is represented in terms of the normalization function

$$\langle n_x\rangle = \frac{\lambda^2}{r}\frac{B(-L,x-2,\zeta)B(x+2,L,\zeta)}{B(-L,L,\zeta)},$$

for odd $x$. The expression for even $x$ is also easily obtained as a closed but complicated form. We have bounds $l\le\langle n_x\rangle\le u$ with some positive constants $l$ and $u$ less than 1. Therefore, these bounds and eq. (10) guarantee the unique domain wall center at $x=\zeta$. The numerical solution of the recursion relation for $B(-L,x,\zeta)$ is useful for seeing the profile of the domain wall practically. The spin one point function for $\langle S_x^{(3)}\rangle$ is depicted in Fig.2.

Now, we study the stability of the domain wall and the spiral structure of the ground state against a band bending perturbation in a variational argument. To bend the lower flat band, we consider the following perturbation

$$H'_{\mathrm{hop}} = -s\sum_{x,\sigma}a_{x\sigma}^\dagger a_{x\sigma}, \tag{15}$$

with a positive small constant $s$. As has been rigorously proved for $q=1$ by Tasaki [3], the all-spin-up state (8) is preserved as a ground state for sufficiently small $s/t$ and $s/U$. Here, we consider the problem also in this limit. The all-spin-up state (8) is an eigenstate of the Hamiltonian $H=H_{\mathrm{hop}}+H_{\mathrm{int}}+H'_{\mathrm{hop}}$ still

$$H|\text{all up}\rangle = E(\text{all up})\ |\text{all up}\rangle,$$

where $E(\text{all up}) = -(L+1)s\epsilon$. If $|q|\neq 1$, other domain wall states (9) are not eigenstates, and the energy expectation values are lower than this energy eigenvalue $E(\text{all up})$. First, we consider the case of $|q|\neq 1$. In the large $t$ and large $U$ limit, the energy expectation value is written in terms of the normalization functions

$$E(\zeta) \equiv \frac{\langle z|H|z\rangle}{\langle z|z\rangle} = E(\text{all up}) - s\sum_{x=-L}^{L}g(x,\zeta), \tag{16}$$

where $x$ is summed over odd integers and

$$\begin{aligned} g(x,\zeta) \equiv& \frac{(|q|^{\frac{1}{2}}-|q|^{-\frac{1}{2}})^2B(-L,x-4,\zeta)}{r^2(|q^{\frac{x-\zeta-2}{2}}|+|q^{-\frac{x-\zeta-2}{2}}|)B(-L,L,\zeta)} \\ &\times\left[\frac{2\epsilon B(x+2,L,\zeta)}{|q^{\frac{x-\zeta}{2}}|+|q^{-\frac{x-\zeta}{2}}|} - \frac{(|q|^{\frac{1}{2}}+|q|^{-\frac{1}{2}})^2B(x+4,L,\zeta)}{r(|q^{\frac{x-\zeta+2}{2}}|+|q^{-\frac{x-\zeta+2}{2}}|)}\right]. \end{aligned} \tag{17}$$

Let us compare the energy expectation values of two solutions with different domain wall centers, namely,$\zeta$ and $\zeta$+2. The analysis of the recursion relation in [10] enables us to estimate $B(-L,x,\zeta)$, then the energy difference of

two nearest neighbor domain walls with a finite distance $\zeta = O(1)$ from the origin is

$$|E(\zeta+2) - E(\zeta)| = O(L|q|^{-L}s).$$

The energy cost by the finite shift of the domain wall center might vanish in the infinite volume limit. If this is true, the domain wall solution with an arbitrary center is stable against the perturbation $H'_{\rm hop}$. The degeneracy corresponding to the location of the domain wall center may be preserved in the infinite volume limit. On the other hand the energy difference between the all-spin-up state and the state with a domain wall at $\zeta = -L+1$ is

$$E(\text{all up}) - E(-L+1) = O(s).$$

The energy eigenvalue of the all-spin-up state is larger than the domain wall state with order 1. Since the energy of the true ground state is lower than the expectation value of the trial state, the all-spin-up state is no longer a ground state unlike the SU(2) invariant model. Therefore, in this variational argument, we conjecture that the localized domain wall structure is stable against this band-bending perturbation. On the other hand, for $|q| = 1$, all the states $|z\rangle$ are still exact eigenstates and are still degenerate to the eigenvalue $E$(all up). Therefore, the stability of the ground states can be proved in the same way as that given by Tasaki [3].

Next, we consider the behavior of one electron added to the quarter filled ground state $|z\rangle$ with a domain wall or a spiral structure,

$$|\psi\rangle \equiv \sum_{x,\sigma} \psi_{x\sigma} c^\dagger_{x\sigma} |z\rangle \tag{18}$$

According to a variational principle, we find the trial wave function $\psi_{x\sigma}$ to optimize the following variational functional

$$\begin{aligned}\langle\psi|H|\psi\rangle &= \sum_{x,y} t^\sigma_{xy} \psi^*_{x\sigma}\psi_{y\sigma} \\ &+ U\sum_x \Bigg( \frac{|z^2q^x|}{1+|z^2q^x|}\psi^*_{x\uparrow}\psi_{x\uparrow} + \frac{1}{1+|z^2q^x|}\psi^*_{x\downarrow}\psi_{x\downarrow} \\ &- \frac{zq^{\frac{x}{2}}}{1+|z^2q^x|}\psi^*_{x\downarrow}\psi_{x\uparrow} - \frac{(zq^{\frac{x}{2}})^*}{1+|z^2q^x|}\psi^*_{x\uparrow}\psi_{x\downarrow}\Bigg)\langle n_x\rangle. \end{aligned} \tag{19}$$

In our model, the scattering of conduction electrons by the domain wall or spiral spins of the lower band has been given already as a well-defined problem. By optimizing this effective energy function under a normalization constraint $\langle\psi|\psi\rangle = 1$, we obtain a two-component Schrödinger equation. At large $\lambda$ or for $|q| = 1$, the $\langle n_x\rangle$ becomes periodic for the lattice unit cells. In particular, at large $\lambda$, eq. (11) implies that a localized spin sits at an odd site and the conduction electron hops mainly on even sites at large $U$. The normalization constraint becomes local in this limit and the hopping term gives a conventional kinetic term in continuum approximation, and the equation for real $q > 1$ becomes that for a conduction electron on the Kondo lattice coupled to the XXZ model obtained by Yamanaka and Koma [11]. The model on the Kondo lattice is realized under special conditions in our model.

In this letter, we construct a set of exact ground states with a ferromagnetic domain wall and a spiral structure in a deformed flat-band Hubbard model. Some results obtained here can be extended to higher dimensional models, as discussed in the original flat-band Hubbard model [2]. After the construction of the domain wall ground state in the XXZ model [5], interesting properties of excitations were discovered [6, 7, 8, 9]. In particular, singular low-lying excitations localized near the domain wall were discussed in arbitrary dimensions [8, 9]. We can expect similar properties of excitations above the domain wall in our electron model as well.

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[1] A. Mielke: J. Phys. A **24** (1991) L73.
[2] H. Tasaki: Phys. Rev. Lett. **69** (1992) 1608.
[3] H. Tasaki: Phys. Rev, Lett. **75** (1995) 4678.
[4] A. Tanaka and H. Ueda: Phys. Rev. Lett. **90** (2003) 067204.
[5] F. C. Alcaraz, S. R. Salinas and W. F. Wreszinski: Phys. Rev. Lett. **75** (1995) 930.
[6] T. Koma and B. Nachtergaele: Lett. Math. Phys. **40** (1997) 1.
[7] T. Koma and B. Nachtergaele: Adv. Theor. Math. Phys. **2** (1998) 533.
[8] T. Matsui: Lett. Math. Phys. **37** (1996) 397.
[9] T. Koma, B. Nachtergaele and S. Starr: Preprint, math-ph/0110017.
[10] M. Homma and C. Itoi: in preparation.
[11] M. Yamanaka and T. Koma: J. Magn. Soc. Jpn. **23** (1999) 141.